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The efficiency of second derivative multistep methods for the numerical integration of stiff systems

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Abstract

A substantial increase in efficiency is achieved by the numerical integration methods which take advantage of the second derivative terms of the differential equation to be solved. The second-derivative of high order accuracy methods are stable, convergent and hence suitable for the numerical integration of stiff systems of initial value problems in ordinary differential equations. The unique feature of the paper is the idea of using all the set of collocation points as additional interpolation points. This desirable feature of the proposed approach actually widens the applicability of the methods, to include many other types of numerical integration methods and has many advantages, including didactic advantages. Furthermore, in this formulation symmetry is retained naturally by the integration identities as equal areas under the various segments of the solution curves over the integration interval. In this way the problem of overlap of solution models usually associated with multistep finite difference methods is overcome. The applications of the second derivative multistep integration methods on a significant class of problems found in the literature produce accurate solutions with low computational cost. Comparison of the efficiency curves obtained seems to be in better agreement with the exact solutions.

Keywords: Block method; Continuous scheme; Second-derivative method; Stiff systems

1. Introduction

We discuss the design principles that lead us to develop efficient methods of high order accuracy with less number of stages and, consequently, reduced computational cost for a given problem, particularly stiff systems of initial value problem in ordinary differential equations given by

$$\frac{dy}{dx} = f(x, y(x)), \qquad y(x_0) = y_0, \quad a \le x \le b, \tag{1.1}$$

where $y : [a, b] \to R^m$ and $f : [a, b] \times R^m \to R^m$ is continuous and differentiable. An equidistant set of points is defined on the integration interval $\Omega : a = x_0 < x_{n+1} < x_{n+2} < \cdots < x_{n+4} = b$, $x_n : x_n = x_0 + nh$,

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$n = 0, 1, \ldots, N-1, h = x_{n+1} - x_n, N = (b-a)/h$. The step size h can either be a variable or constant, it is assumed in this paper as a constant on the partition Ω, N is a positive integer. Many of the existing numerical integration methods considered for the numerical solution of (1.1) are of low orders and not suitable for large stiff systems of initial value problems in ordinary differential equations. Some were derived on the basis that the required function evaluations are to be done only at the grid points as well as at the first derivative of the differential equation. This is because we are familiar with solution at the grid-points, which is typically of discrete variable methods (Euler method, Runge–Kutta methods, Picard method, etc.) Henrici [1]. Earlier, some authors considered the introduction of off-grid points in between the familiar grid points (see [2–5]), with the hope of generalizing the two traditional numerical integration methods (Runge–Kutta methods and linear multistep methods) as a consequence of the barrier theorem of Dahlquist [6]. Similarly, many authors had introduced the second derivative terms in their methods for example, see [7–15]. In this report, we consider methods that are suitable for generating the solution of stiff systems of initial value problems at both grid and off-grid points simultaneously within the integration interval. These methods are derived by using all the set of collocation points as additional interpolation points in the numerical schemes.

Like traditional Runge–Kutta methods, second-derivative block multistep collocation integrators admit the addition of extra stages, which introduce extra degrees of freedom that can be used to increase the order of accuracy or modify the region of absolute stability. Second-derivative block multistep integrators permit the evaluation of higher derivatives of the unknown in order to decrease the memory footprint and communication overhead. Block methods generally, preserve the traditional advantages of one-step methods (Runge–Kutta methods, Taylor series method, Picard method etc.) of being self-starting and of permitting easy change of step length during integration (see Lambert [16]). Their advantage over Runge–Kutta methods lies in the fact that they are less expensive in terms of number of function evaluations per step. In this paper, we derive a new class of second-derivative block multistep methods with high order of accuracy, very low error constants, large regions of absolute stability, which behave essentially like one-step methods and converge rapidly to the required solution.

Definition 1.1. A numerical method is said to be A-stable if its region of absolute stability contains the whole of the complex left hand-half plane $\mathrm{Re}\, h\lambda < 0$ (see, Dahlquist [6]). Alternatively, a numerical method is called A-stable if all the solution of (1.1) tend to zero as $n \to \infty$, when the method is applied with fixed positive h to any differential equation of the form $dy/dx = \lambda y$, where λ is a complex constant with negative real part.

Definition 1.2. A numerical method is said to be $A(\alpha)$-stable, $\alpha \in (0, \pi/2)$ if its region of absolute stability contains the infinite wedge $W_\alpha = \{\lambda h : -\alpha < \pi - \arg(\lambda h) < \alpha\}$.

Definition 1.3. A solution $y(x)$ of (1.1) is said to be stable if given any $\epsilon > 0$ there is $\delta > 0$ such that any other solution $\hat{y}(x)$ of (1.1) which satisfies

$$\left|y(a) - \hat{y}(a)\right| \le \delta \tag{1.2a}$$

also satisfies

$$\left|y(x) - \hat{y}(x)\right| \le \epsilon \tag{1.2b}$$

for all $x > a$.

The solution $y(x)$ is asymptotically stable if in addition to (1.2b) $\left|y(x) - \hat{y}(x)\right| \to 0$ as $x \to \infty$.

Definition 1.4. Let Y_m and F_m be defined by $Y_m = (y_n, y_{n+1}, \ldots, y_{n+r-1})^T$, $F_m = (f_n, f_{n+1}, \ldots, f_{n+r-1})^T$. Then a general k-block, r-point block method is a matrix of finite difference equation of the form

$$Y_m = \sum_{j=1}^{k} A_i Y_{m-i} + h \sum_{i=0}^{k} B_i F_{m-i}, \tag{1.3}$$

where all the A_i's and B_i's are properly chosen $r \times r$ matrix coefficients and $m = 0, 1, 2, \ldots,$ represents the block number, $n = mr$ is the first step number of the mth block and r is the proposed block size [17].

2. Derivation of the second derivative multistep methods

The main aim of this section is to present the general derivation principle of the special class of methods for the solution of stiff systems of initial value problems. We shall do this through the interpolation and collocation of a polynomial on equi-distant step-points $\{x_j\}$ where the interpolation polynomial is of the form,

$$y(x) = \phi_0 + \phi_1 x + \phi_2 x^2 + \cdots + \phi_{p-1} x^{p-1} = \sum_{i=0}^{p-1} \phi_i x^i \tag{2.1}$$

which is twice-continuously differentiable. We set the sum $r + s + t$ to be equal to p so as to be able to determine $\{\phi_i\}$ uniquely. We interpolate $y(x)$ at the points $\{x_{n+j}\}$ and collocate at the points $\{c_{n+j}\}$ to obtain the following equations,

$$y(x_{n+j}) = y_{n+j}, \quad (j = 0, 1, \ldots, r-1), \tag{2.2}$$

$$y'(c_{n+j}) = f_{n+j}, \quad (j = 0, 1, \ldots, s-1), \tag{2.3}$$

$$y''(c_{n+j}) = g_{n+j}, \quad (j = 0, 1, \ldots, t-1). \tag{2.4}$$

Here y_{n+j} is the interpolation data of $y(x)$ on $\{x_{n+j}\}$ and f_{n+j}, g_{n+j} are the collocation data of $y'(x)$ and $y''(x)$ on $\{c_{n+j}\}$ respectively. In the spirit of Mitsui and Yakubu [18], Eqs. (2.2)–(2.4) can be expressed in the matrix–vector form as:

$$V\phi = y \tag{2.5}$$

where the p-square matrix V, the p-vectors ϕ, and y are defined as follows,

$$V = \begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & \cdots & x_n^{p-1} \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & x_{n+1}^4 & \cdots & x_{n+1}^{p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n+r-1} & x_{n+r-1}^2 & x_{n+r-1}^3 & x_{n+r-1}^4 & \cdots & x_{n+r-1}^{p-1} \\ 0 & 1 & 2c_n & 3c_n^2 & 4c_n^3 & \cdots & D'c_n^{p-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 2c_{n+s-1} & 3c_{n+s-1}^2 & 4c_{n+s-1}^3 & \cdots & D'c_{n+s-1}^{p-2} \\ 0 & 0 & 2 & 6c_n & 12c_n^2 & \cdots & D''c_n^{p-3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 2 & 6c_{n+t-1} & 12c_{n+t-1}^2 & \cdots & D''c_{n+t-1}^{p-3} \end{pmatrix} \tag{2.6}$$

$$\phi = \left(\phi_0, \phi_1, \phi_2, \ldots, \phi_{p-1}\right)^T, \qquad y = \left(y_n, \ldots, y_{n+r-1}, f_n, \ldots, f_{n+s-1}, g_n, \ldots, g_{n+t-1}\right)^T, \tag{2.7}$$

where $D' = (p-1)$ and $D'' = (p-1)(p-2)$ represent the first and second derivatives with respect to x. Similar to the Vandermonde matrix, V in (2.5) is non-singular. A closed form of the solution for the system (2.5) is presented which has been obtained by considering the inverse of the Vandermonde matrix, that is,

$$\phi = My \quad \text{where } M = V^{-1}. \tag{2.8}$$

The interpolation polynomial $y(x)$ in (2.1) and the Eqs. (2.2)–(2.4) can be rearranged to obtain the multistep collocation method of Onumanyi et al. [19] which was a generalization of Lie and Nørsett [20] and now extend to second derivative as follows

$$y(x) = \sum_{j=0}^{r-1} \phi_j(x) y_{n+j} + h \sum_{j=0}^{s-1} \psi_j(x) f_{n+j} + h^2 \sum_{j=0}^{t-1} \gamma_j(x) g_{n+j} \tag{2.9}$$

where

$$y_{n+j} \approx y\left(x_n + jh\right), \qquad f_{n+j} \equiv f\left(x_n + jh, y\left(x_n + jh\right)\right) \quad \text{and} \quad g_{n+j} \equiv \left.\frac{df\left(x, y\left(x\right)\right)}{dx}\right|_{\substack{x = x_{n+j} \\ y = y_{n+j}}}.$$

Here the continuous coefficients $\phi_j(x)$, $\psi_j(x)$ and $\gamma_j(x)$ are polynomials of degree $(p-1)$ given by

$$\phi_j(x) = \sum_{i=0}^{p-1} \phi_{j,i+1} x^i, \qquad h\psi_j(x) = h \sum_{i=0}^{p-1} \psi_{j,i+1} x^i \quad \text{and} \quad h^2\gamma_j(x) = h^2 \sum_{j=0}^{p-1} \gamma_{j,i+1} x^i. \tag{2.10}$$

In fact, the above coefficients can be obtained from the components of the matrix V^{-1}. That is, if the identity

$$M = \begin{pmatrix} \phi_0^{(0)} & \phi_0^{(1)} & \cdots & \phi_0^{(r-1)} & h\psi_0^{(0)} & \cdots & h\psi_0^{(s-1)} & h^2\gamma_0^{(0)} & \cdots & h^2\gamma_0^{(t-1)} \\ \phi_1^{(0)} & \phi_1^{(1)} & \cdots & \phi_1^{(r-1)} & h\psi_1^{(0)} & \cdots & h\psi_1^{(s-1)} & h^2\gamma_1^{(0)} & \cdots & h^2\gamma_1^{(t-1)} \\ \phi_2^{(0)} & \phi_2^{(1)} & \cdots & \phi_2^{(r-1)} & h\psi_2^{(0)} & \cdots & h\psi_2^{(s-1)} & h^2\gamma_2^{(0)} & \cdots & h^2\gamma_2^{(t-1)} \\ \phi_3^{(0)} & \phi_3^{(1)} & \cdots & \phi_3^{(r-1)} & h\psi_3^{(0)} & \cdots & h\psi_3^{(s-1)} & h^2\gamma_3^{(0)} & \cdots & h^2\gamma_3^{(t-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \phi_{p-1}^{(0)} & \phi_{p-1}^{(1)} & \cdots & \phi_{p-1}^{(r-1)} & h\psi_{p-1}^{(0)} & \cdots & h\psi_{p-1}^{(s-1)} & h^2\gamma_{p-1}^{(0)} & \cdots & h^2\gamma_{p-1}^{(t-1)} \end{pmatrix} = V^{-1} \tag{2.11}$$

holds. The choice $M = V^{-1}$ leads to the determination of the numerical constant coefficients $\phi_{j,i+1}$, $\psi_{j,i+1}$ and $\gamma_{j,i+1}$ in (2.10). Actual evaluations of matrices M and V are carried out with a computer algebra system, for example, Maple software.

3. A tenth order second derivative multistep method

The parameters of the first second-derivative method can now be obtained by considering the multistep collocation method (2.9). We define $\xi = (x - x_n)$ which we shall use in the continuous scheme of the second-derivative method. Thus, expanding (2.9) we have the following continuous scheme:

$$\begin{aligned} y(x) = {} & \phi_0(x)y_n + h[\psi_0(x)f_n + \psi_1(x)f_{n+1} + \psi_2(x)f_{n+2} + \psi_3(x)f_{n+3} + \psi_4(x)f_{n+4}] \\ & + h^2[\gamma_0(x)g_n + \gamma_1(x)g_{n+1} + \gamma_2(x)g_{n+2} + \gamma_3(x)g_{n+3} + \gamma_4(x)g_{n+4}] \end{aligned} \tag{3.1}$$

where

$$\phi_0(x) = 1,$$

$$\psi_0(x) = \left[\frac{\begin{array}{c}3150\xi^{10} - 69160h\xi^9 + 650475h^2\xi^8 - 3416400h^3\xi^7 + 10925250h^4\xi^6 \\ - 21637224h^5\xi^5 + 25395300h^6\xi^4 - 14666400h^7\xi^3 + 4354560h^9\xi\end{array}}{4354560h^9}\right],$$

$$\psi_1(x) = \left[\frac{\begin{array}{c}1260\xi^{10} - 25760h\xi^9 + 220815h^2\xi^8 - 1024560h^3\xi^7 + 2760240h^4\xi^6 \\ - 4261824h^5\xi^5 + 3386880h^6\xi^4 - 967680h^7\xi^3\end{array}}{272160h^9}\right],$$

$$\psi_2(x) = \left[\frac{\begin{array}{c}35\xi^9 - 630h\xi^8 + 4590h^2\xi^7 - 17220h^3\xi^6 + 34839h^4\xi^5 - 35910h^5\xi^4 \\ + 15120h^6\xi^3\end{array}}{5040h^8}\right],$$

$$\psi_3(x) = \left[\frac{\begin{array}{c}-1260\xi^{10} + 24640h\xi^9 - 200655h^2\xi^8 + 880560h^3\xi^7 - 2249520h^4\xi^6 \\ +3358656h^5\xi^5 - 2741760h^6\xi^4 + 967680h^7\xi^3\end{array}}{272160h^9}\right],$$

$$\psi_4(x) = \left[\frac{\begin{array}{c}-3150\xi^{10} + 56840h\xi^9 - 428715h^2\xi^8 + 1754640h^3\xi^7 - 4218690h^4\xi^6 \\ +5987016h^5\xi^5 - 4690980h^6\xi^4 + 1602720h^7\xi^3\end{array}}{4354560h^9}\right],$$

$$\gamma_0(x) = \left[\frac{\begin{array}{c}126\xi^{10} - 2800h\xi^9 + 26775h^2\xi^8 - 144000h^3\xi^7 + 477330h^4\xi^6 \\ -1002960h^5\xi^5 + 1316700h^6\xi^4 - 1008000h^7\xi^3 + 362880h^8\xi\end{array}}{725760h^8}\right],$$

$$\gamma_1(x) = \left[\frac{\begin{array}{c}252\xi^{10} - 5320h\xi^9 + 47565h^2\xi^8 - 233640h^3\xi^7 + 682080h^4\xi^6 \\ -1187424h^5\xi^5 + 1149120h^6\xi^4 - 483840h^7\xi^3\end{array}}{90720h^8}\right],$$

$$\gamma_2(x) = \left[\frac{\begin{array}{c}2\xi^{10} - 40h\xi^9 + 335h^2\xi^8 - 1520h^3\xi^7 + 4030h^4\xi^6 - 648h^5\xi^5 \\ +5280h^6\xi^4 - 1920h^7\xi^3\end{array}}{320h^8}\right],$$

$$\gamma_3(x) = \left[\frac{\begin{array}{c}252\xi^{10} - 4760h\xi^9 + 37485h^2\xi^8 - 159480h^3\xi^7 + 396480h^4\xi^6 \\ -578592h^5\xi^5 + 463680h^6\xi^4 - 161280h^7\xi^3\end{array}}{90720h^8}\right],$$

$$\gamma_4(x) = \left[\frac{\begin{array}{c}126\xi^{10} - 2240h\xi^9 + 16695h^2\xi^8 - 67680h^3\xi^7 + 161490h^4\xi^6 \\ -227808h^5\xi^5 + 177660h^6\xi^4 - 60480h^7\xi^3\end{array}}{725760h^8}\right].$$

Evaluating the continuous scheme $y(x)$ in (3.1) at the points $\{x_{n+1}, x_{n+2}, x_{n+3}, x_{n+4}\}$ we obtain the first block second derivative of high-order accuracy method, consisting of four members in a block as follows:

$$\begin{aligned}
y_{n+1} &= y_n + \frac{h}{4354560}[1539551 f_n + 1429936 f_{n+1} + 711936 f_{n+2} + 613456 f_{n+3} + 59681 f_{n+4}] \\
&\quad + \frac{h^2}{725760}[26051 g_n - 249656 g_{n+1} - 183708 g_{n+2} - 49720 g_{n+3} - 2237 g_{n+4}] \qquad (3.2)\\
y_{n+2} &= y_n + \frac{h}{68040}[24463 f_n + 52928 f_{n+1} + 44928 f_{n+2} + 12608 f_{n+3} + 1153 f_{n+4}] \\
&\quad + \frac{h^2}{11340}[421 g_n - 3040 g_{n+1} - 4536 g_{n+2} - 992 g_{n+3} - 43 g_{n+4}] \\
y_{n+3} &= y_n + \frac{h}{17920}[6501 f_n + 14736 f_{n+1} + 20736 f_{n+2} + 11376 f_{n+3} + 411 f_{n+4}] \\
&\quad + \frac{h^2}{8960}[339 g_n - 2232 g_{n+1} - 2268 g_{n+2} - 1464 g_{n+3} - 45 g_{n+4}] \\
y_{n+4} &= y_n + \frac{h}{8505}[3202 f_n + 8192 f_{n+1} + 11232 f_{n+2} + 8192 f_{n+3} + 3202 f_{n+4}] \\
&\quad + \frac{h^2}{2835}[116 g_n - 512 g_{n+1} + 512 g_{n+3} - 116 g_{n+4}].
\end{aligned}$$

3.1. A fourteenth order upgraded second derivative multistep method

To upgrade (see [21,22]) the second-derivative of high-order accuracy method (3.2), we consider the inclusion of all the set of collocation points as additional interpolation points. Hence expanding (2.9) we obtain,

$$\begin{aligned} y(x) &= \phi_0(x)y_n + \phi_1(x)y_{n+1} + \phi_2(x)y_{n+2} + \phi_3(x)y_{n+3} + \phi_4(x)y_{n+4} \\ &\quad + h[\psi_0(x)f_n + \psi_1(x)f_{n+1} + \psi_2(x)f_{n+2} + \psi_3(x)f_{n+3} + \psi_4(x)f_{n+4}] \\ &\quad + h^2[\gamma_0(x)g_n + \gamma_1(x)g_{n+1} + \gamma_2(x)g_{n+2} + \gamma_3(x)g_{n+3} + \gamma_4(x)g_{n+4}] \end{aligned} \tag{3.3}$$

where

$$\phi_0(x) = \left[\frac{\begin{array}{c}260\xi^{14} - 7725h\xi^{13} + 103062h^2\xi^{12} - 814985h^3\xi^{11} + 4245330h^4\xi^{10} - 15304875h^5\xi^9 + 39010114h^6\xi^8 \\ - 70444155h^7\xi^7 + 88636410h^8\xi^6 - 74476900h^9\xi^5 + 38046936h^{10}\xi^4 - 9159360h^{11}\xi^3 + 165888h^{14}\end{array}}{165888h^{14}}\right],$$

$$\phi_1(x) = \left[\frac{\begin{array}{c}-40\xi^{14} + 1145h\xi^{13} - 14626h^2\xi^{12} + 109902h^3\xi^{11} - 538956h^4\xi^{10} + 180820h^5\xi^9 - 4227722h^6\xi^8 \\ + 6876628h^7\xi^7 - 7614680h^8\xi^6 + 5464224h^9\xi^5 - 2291328h^{10}\xi^4 + 428544h^{11}\xi^3\end{array}}{1296h^{14}}\right],$$

$$\phi_2(x) = \left[\frac{\begin{array}{c}15\xi^{14} - 420h\xi^{13} + 5239h^2\xi^{12} - 38376h^3\xi^{11} + 183141h^4\xi^{10} - 596900h^5\xi^9 + 1353333h^6\xi^8 \\ - 2130384h^7\xi^7 + 2277280h^8\xi^6 - 1571328h^9\xi^5 + 628992h^{10}\xi^4 - 110592h^{11}\xi^3\end{array}}{256h^{14}}\right],$$

$$\phi_3(x) = \left[\frac{\begin{array}{c}-40\xi^{14} + 1095h\xi^{13} - 13326h^2\xi^{12} + 95026h^3\xi^{11} - 440484h^4\xi^{10} + 1391475h^5\xi^9 - 3052022h^6\xi^8 \\ + 4641324h^7\xi^7 - 4789800h^8\xi^6 + 3191648h^9\xi^5 - 1235328h^{10}\xi^4 + 210432h^{11}\xi^3\end{array}}{1296h^{14}}\right],$$

$$\phi_4(x) = \left[\frac{\begin{array}{c}260\xi^{14} - 6835h\xi^{13} + 79922h^2\xi^{12} - 548151h^3\xi^{11} + 2447622h^4\xi^{10} - 7462965h^5\xi^9 + 15837334h^6\xi^8 \\ - 23364869h^7\xi^7 + 23459590h^8\xi^6 - 15254172h^9\xi^5 + 5778216h^{10}\xi^4 - 965952h^{11}\xi^3\end{array}}{165888h^{14}}\right],$$

$$\psi_0(x) = \left[\frac{\begin{array}{c}25\xi^{14} - 746h\xi^{13} + 10005h^2\xi^{12} - 79630h^3\xi^{11} + 418175h^4\xi^{10} - 1523262h^5\xi^9 + 3935615h^6\xi^8 \\ - 7238290h^7\xi^7 + 9345300h^8\xi^6 - 8159288h^9\xi^5 + 4434880h^{10}\xi^4 - 1198080h^{11}\xi^3 + 55296h^{13}\xi\end{array}}{55296h^{13}}\right],$$

$$\psi_1(x) = \left[\frac{\begin{array}{c}-5\xi^{14} + 143h\xi^{13} - 1824h^2\xi^{12} + 13674h^3\xi^{11} - 66813h^4\xi^{10} + 222891h^5\xi^9 - 516550h^6\xi^8 \\ + 828604h^7\xi^7 - 897432h^8\xi^6 + 621216h^9\xi^5 - 245376h^{10}\xi^4 + 41472h^{11}\xi^3\end{array}}{432h^{13}}\right],$$

$$\psi_2(x) = \left[\frac{\begin{array}{c}\xi^{13} - 26h\xi^{12} + 297h^2\xi^{11} - 1958h^3\xi^{10} + 8227h^4\xi^9 - 22950h^5\xi^8 + 42907h^6\xi^7 \\ - 52922h^7\xi^6 + 41112h^8\xi^5 - 18144h^9\xi^4 + 3456h^{10}\xi^3\end{array}}{64h^{12}}\right],$$

$$\psi_3(x) = \left[\frac{\begin{array}{c}5\xi^{14} - 137h\xi^{13} + 1668h^2\xi^{12} - 11894h^3\xi^{11} + 55109h^4\xi^{10} - 173949h^5\xi^9 + 381130h^6\xi^8 \\ - 578884h^7\xi^7 + 596616h^8\xi^6 - 397024h^9\xi^5 + 153472h^{10}\xi^4 - 26112h^{11}\xi^3\end{array}}{432h^{13}}\right],$$

$$\psi_4(x)=\left[\frac{\begin{array}{c}-25\xi^{14}+654h\xi^{13}-7613h^2\xi^{12}+52002h^3\xi^{11}-231351h^4\xi^{10}+703098h^5\xi^9-1487735h^6\xi^8\\+2189262h^7\xi^7-2193244h^8\xi^6+1423368h^9\xi^5-538272h^{10}\xi^4+89856h^{11}\xi^3\end{array}}{55296h^{13}}\right],$$

$$\gamma_0(x)=\left[\frac{\begin{array}{c}\xi^{14}-30h\xi^{13}+405h^2\xi^{12}-3250h^3\xi^{11}+17247h^4\xi^{10}-63690h^5\xi^9+167615h^6\xi^8-316350h^7\xi^7\\+424428h^8\xi^6-394280h^9\xi^5+240480h^{10}\xi^4-86400h^{11}\xi^3+13824h^{12}\xi^2\end{array}}{27648h^{12}}\right],$$

$$\gamma_1(x)=\left[\frac{\begin{array}{c}-\xi^{14}+29h\xi^{13}-376h^2\xi^{12}+2874h^3\xi^{11}-14373h^4\xi^{10}+49317h^5\xi^9-118298h^6\xi^8\\+198052h^7\xi^7-226376h^8\xi^6+167904h^9\xi^5-72576h^{10}\xi^4+13824h^{11}\xi^3\end{array}}{432h^{12}}\right],$$

$$\gamma_2(x)=\left[\frac{\begin{array}{c}\xi^{14}-28h\xi^{13}+349h^2\xi^{12}-2552h^3\xi^{11}+12143h^4\xi^{10}-39404h^5\xi^9+88807h^6\xi^8\\-138736h^7\xi^7+146956h^8\xi^6-100368h^9\xi^5+39744h^{10}\xi^4-6912h^{11}\xi^3\end{array}}{128h^{12}}\right],$$

$$\gamma_3(x)=\left[\frac{\begin{array}{c}-\xi^{14}+27h\xi^{13}-324h^2\xi^{12}+2278h^3\xi^{11}-10413h^4\xi^{10}+32451h^5\xi^9-70262h^6\xi^8x\\+105564h^7\xi^7-107736h^8\xi^6+71072h^9\xi^5-27264h^{10}\xi^4+4608h^{11}\xi^3\end{array}}{432h^{12}}\right],$$

$$\gamma_4(x)=\left[\frac{\begin{array}{c}\xi^{14}-26h\xi^{13}+301h^2\xi^{12}-2046h^3\xi^{11}+9063h^4\xi^{10}-27438h^5\xi^9+57863h^6\xi^8\\-84898h^7\xi^7+84836h^8\xi^6-54936h^9\xi^5+20736h^{10}\xi^4-3456h^{11}\xi^3\end{array}}{27648h^{12}}\right].$$

Evaluating the continuous scheme $y(x)$ in (3.3) at the points $\{x_{n+u}, x_{n+v}, x_{n+w}, x_{n+q}\}$ where u, v, w and q are respectively $\left\{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}\right\}$ we obtain the first, third, fifth and seventh members in the block (3.4). Differentiating the continuous scheme in (3.3) once, evaluate at the points $\{x_{n+u}, x_{n+v}, x_{n+w}, x_{n+q}\}$ and solve simultaneously for the values of $\{y_{n+1}, y_{n+2}, y_{n+3}, y_{n+4}\}$ to complete the block second-derivative of high-order accuracy method, consisting of eight members:

$$\begin{aligned}
y_{n+u} &= \frac{9818375}{50331648}y_n+\frac{728875}{393216}y_{n+1}-\frac{6474125}{4194304}y_{n+2}+\frac{201341}{393216}y_{n+3}-\frac{864875}{50331648}y_{n+4}\\
&\quad+\frac{h}{33554432}[1414875f_n+5488000f_{n+1}+8232000f_{n+2}-6366080f_{n+3}+160125f_{n+4}]\\
&\quad+\frac{h^2}{16777216}[42875g_n+2744000g_{n+1}-3087000g_{n+2}+548800g_{n+3}-6125g_{n+4}] \qquad (3.4)\\
y_{n+1} &= -\frac{257211}{342144}y_n+\frac{477}{176}y_{n+2}-\frac{295}{297}y_{n+3}+\frac{49}{1408}y_{n+4}\\
&\quad+\frac{h}{15523200}[-2314025f_n-8388608f_{n+u}-13798400f_{n+1}\\
&\quad-5605600f_{n+2}+5732608f_{n+3}-150475f_{n+4}]\\
&\quad+\frac{h^2}{7761600}[-64925g_n-1411200g_{n+1}+2616600g_{n+2}-501760g_{n+3}+5775g_{n+4}]\\
y_{n+v} &= \frac{-59125}{16777216}y_n+\frac{52875}{131072}y_{n+1}+\frac{2824875}{4194304}y_{n+2}-\frac{9875}{131072}y_{n+3}+\frac{32841}{16777216}y_{n+4}\\
&\quad+\frac{h}{33554432}[-31125f_n+3888000f_{n+1}-5832000f_{n+2}+912000f_{n+3}-17955f_{n+4}]\\
&\quad+\frac{h^2}{16777216}[-1125g_n+216000g_{n+1}+729000g_{n+2}-72000g_{n+3}+675g_{n+4}]
\end{aligned}$$

$$
\begin{aligned}
y_{n+2} &= -\frac{2359}{647352}y_n + \frac{9136}{8991}y_{n+1} - \frac{1072}{80919}y_{n+3} + \frac{55}{71928}y_{n+4} \\
&\quad + \frac{h}{16183800}[-15025 f_n + 3974400 f_{n+1} - 8388608 f_{n+v} + 4082400 f_{n+2} \\
&\quad + 89600 f_{n+3} - 3483 f_{n+4}] \\
&\quad + \frac{h^2}{8091900}[-525 g_n + 172800 g_{n+1} - 145800 g_{n+2} - 9600 g_{n+3} + 135 g_{n+4}] \\
y_{n+w} &= \frac{32841}{16777216}y_n - \frac{9875}{131072}y_{n+1} + \frac{2824875}{4194304}y_{n+2} + \frac{52875}{131072}y_{n+3} - \frac{59125}{16777216}y_{n+4} \\
&\quad + \frac{h}{33554432}[17955 f_n - 912000 f_{n+1} + 5832000 f_{n+2} - 3888000 f_{n+3} + 31125 f_{n+4}] \\
&\quad + \frac{h^2}{16777216}[675 g_n - 72000 g_{n+1} + 729000 g_{n+2} + 216000 g_{n+3} - 1125 g_{n+4}] \\
y_{n+3} &= -\frac{55}{73088}y_n + \frac{67}{5139}y_{n+1} + \frac{8991}{9136}y_{n+2} + \frac{2359}{657792}y_{n+4} \\
&\quad + \frac{h}{16444800}[-3483 f_n + 89600 f_{n+1} + 4082400 f_{n+2} - 8388608 f_{n+w} \\
&\quad +3974400 f_{n+3} - 15025 f_{n+4}] \\
&\quad + \frac{h^2}{8222400}[-135 g_n + 9600 g_{n+1} + 145800 g_{n+2} - 172800 g_{n+3} + 525 g_{n+4}] \\
y_{n+q} &= \frac{-864875}{50331648}y_n + \frac{201341}{393216}y_{n+1} - \frac{6474125}{4194304}y_{n+2} + \frac{728875}{393216}y_{n+3} + \frac{9818375}{50331648}y_{n+4} \\
&\quad + \frac{h}{33554432}[-160125 f_n + 6366080 f_{n+1} - 8232000 f_{n+2} - 5488000 f_{n+3} - 1414875 f_{n+4}] \\
&\quad + \frac{h^2}{16777216}[-6125 g_n + 548800 g_{n+1} - 3087000 g_{n+2} + 2744000 g_{n+3} + 42875 g_{n+4}] \\
y_{n+4} &= \frac{1323}{28579}y_n - \frac{37760}{28579}y_{n+1} + \frac{103032}{28579}y_{n+2} - \frac{38016}{28579}y_{n+3} \\
&\quad + \frac{h}{35009275}[451425 f_n - 17197824 f_{n+1} + 16816800 f_{n+2} \\
&\quad + 41395200 f_{n+3} + 25165824 f_{n+q} + 6942075 f_{n+4}] \\
&\quad + \frac{h^2}{35009275}[34650 g_n - 3010560 g_{n+1} + 15699600 g_{n+2} - 8467200 g_{n+3} - 389550 g_{n+4}].
\end{aligned}
$$

The methods so derived consist of some members in a block and give in general more accurate approximations to the exact solution than the Adam's family of methods. They have smaller error constants compared to the traditional methods of the same order in current use (Runge–Kutta and Linear multistep methods). Thus, the price for this higher accuracy is that $\{y_{n+u}, y_{n+1}, y_{n+v}, \ldots, y_{n+4}\}$ are only defined implicitly by the methods in the block. Therefore in their applications to solve ordinary differential equations, a nonlinear equation has to be solved at each time step.

4. Analysis of the properties of the second derivative multistep methods

4.1. Order, consistency, zero-stability and convergence of the SDMMs

With the multistep collocation method (2.9) we associate the linear difference operator ℓ defined by

$$\ell[y(x); h] = \sum_{j=0}^{r} \phi_j(x) y(x + jh) + h \sum_{j=0}^{s} \psi_j(x) y'(x + jh) + h^2 \sum_{j=0}^{t} \gamma_j(x) y''(x + jh) \tag{4.1}$$

where $y(x)$ is an arbitrary function, continuously differentiable on $[a, b]$. Following Lambert [16] and Fatunla [23], we can write the terms in (4.1) as a Taylor series expansion about the point x to obtain the expression,

$$\ell[y(x); h] = C_0 y(x) + C_1 h y'(x) + C_2 h^2 y''(x) + \cdots + C_p h^p y^p(x) + \cdots, \tag{4.2}$$

Table 1
Order and error constants of the second derivative multistep methods.

Method	Order	Error constant
Block method (3.2)	(i) $P = 10$	$C_{11} = 1.7528 \times 10^{-6}$
	(ii) $P = 10$	$C_{11} = 2.0359 \times 10^{-6}$
	(iii) $P = 10$	$C_{11} = 2.3191 \times 10^{-6}$
	(iv) $P = 10$	$C_{11} = 4.0719 \times 10^{-6}$
Block method (3.4)	(i) $P = 14$	$C_{15} = 2.7015 \times 10^{-11}$
	(ii) $P = 14$	$C_{15} = -1.0960 \times 10^{-10}$
	(iii) $P = 14$	$C_{15} = 2.1266 \times 10^{-12}$
	(iv) $P = 14$	$C_{15} = 2.5519 \times 10^{-12}$
	(v) $P = 14$	$C_{15} = 2.1266 \times 10^{-12}$
	(vi) $P = 14$	$C_{15} = 2.5519 \times 10^{-12}$
	(vii) $P = 14$	$C_{15} = 2.7015 \times 10^{-11}$
	(viii) $p = 14$	$C_{15} = 1.0960 \times 10^{-10}$

where the constant coefficients C_p, $p = 0, 1, 2, \ldots$, are given as follows:

$$C_0 = \sum_{j=0}^{r} \phi_j$$

$$C_1 = \sum_{j=1}^{r} j\phi_j - \sum_{j=0}^{s} \psi_j$$

$$C_2 = \frac{1}{2!}\left(\sum_{j=1}^{r} j^2\phi_j - 2\sum_{j=1}^{s} j\psi_j - 2\sum_{j=0}^{t} \gamma_j\right)$$

$$\vdots$$

$$C_p = \frac{1}{p!}\left(\sum_{j=1}^{r} j^p\phi_j - \frac{1}{(p-1)!}\sum_{j=1}^{s} j^{p-1}\psi_j - \frac{1}{(p-2)!}\sum_{j=1}^{t} j^{p-2}\gamma_j\right), \quad p = 3, 4, \ldots.$$

According to Lambert [16], the multistep collocation method (2.9) has order p if

$$\ell\,[y(x); h] = O\left(h^{p+1}\right), \qquad C_0 = C_1 = \cdots = C_p = 0, \qquad C_{p+1} \neq 0. \tag{4.3}$$

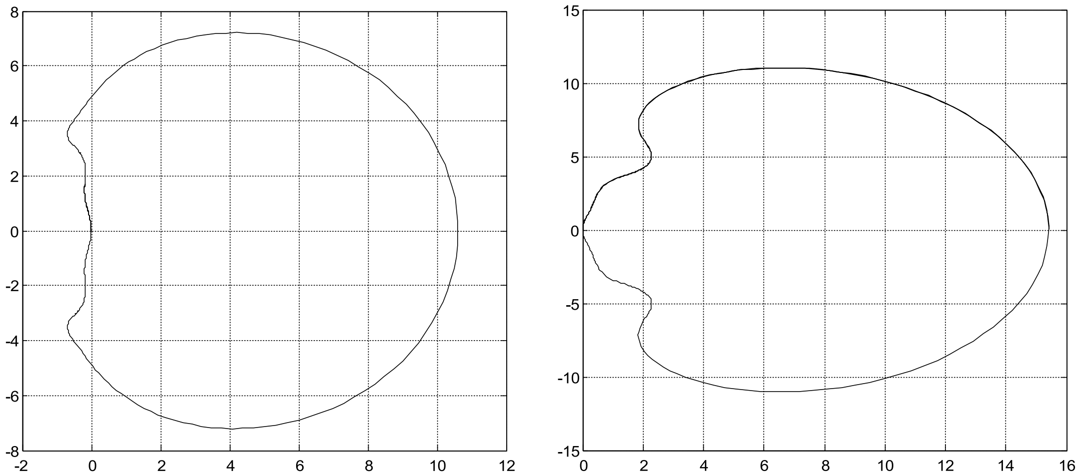
Therefore, C_{p+1} is the error constant and $C_{p+1}h^{p+1}y^{(p+1)}(x_n)$ is the principal local truncation error at the point x_n [12]. Hence, from our calculation the order and error constants for the constructed methods are presented in Table 1. It is clear from the table that the block second-derivative high-order method (3.2) is of order ten. The members of the block second-derivative high-order method (3.4) are of uniformly accurate order. The members of this block method have smaller error constants and hence more accurate than those members of the block method (3.2).

Definition 4.1 (*Consistency*)**.** The block second derivative of high-order accuracy methods (3.2) and (3.4) are said to be consistent if the order of the individual method is greater than or equal to one, that is if $p \geq 1$.

(i) $\rho(1) = 0$ and

(ii) $\rho'(1) = \sigma(1)$, where $\rho(z)$ and $\sigma(z)$ are respectively the 1st and 2nd characteristic polynomials.

From Table 1 we can attest that the members of the block second-derivative high-order accuracy methods are consistent.



Method (3.2) which is A(α)-stable **Method (3.4) which is A-stable**

Fig. 1. Regions of absolute stability of the second derivative multistep methods.

Definition 4.2 (*Zero-Stability*)**.** The block second-derivative high-order methods (3.2) and (3.4) are said to be zero-stable if the roots

$$\rho(\lambda) = \det\left[\sum_{i=0}^{k} A^{(i)}\lambda^{k-i}\right] = 0$$

satisfies $\left|\lambda_j\right| \leq 1,\ j = 1, \ldots, k$ and for those roots with $\left|\lambda_j\right| = 1$, the multiplicity does not exceed 2, Lambert [16].

Definition 4.3 (*Convergence*)**.** The necessary and sufficient conditions for the block second-derivative high-order methods (3.2) and (3.4) to be convergent are that they must be consistent and zero-stable Dahlquist [6]. Hence from Definitions 4.1 and 4.2 the second-derivative high-order methods are convergent.

4.2. Regions of absolute stability of the block second derivative multistep methods

To study the stability properties of the block second-derivative high-order methods we reformulate (3.2) and (3.4) as general linear methods (see Burrage and Butcher [24]). Hence, we use the notation introduced by Butcher [25] in which a general linear method is represented by a partitioned $(s + r) \times (s + r)$ matrix, (containing A, U, B, V),

$$\begin{bmatrix} Y^{[n]} \\ y^{[n-1]} \end{bmatrix} = \left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \begin{bmatrix} hf\left(Y^{[n]}\right) \\ y^{[n]} \end{bmatrix}, \quad n = 1, 2, \ldots, N, \tag{4.4a}$$

where

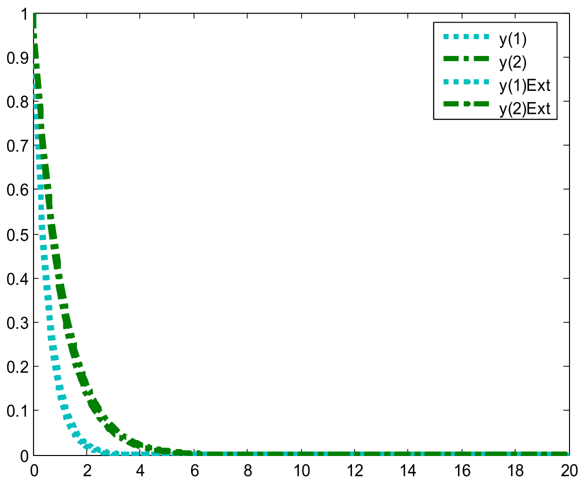
$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \qquad y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \qquad f\left(Y^{[n]}\right) = \begin{bmatrix} f(Y_1^{[n]}) \\ f(Y_2^{[n]}) \\ \vdots \\ f(Y_s^{[n]}) \end{bmatrix}, \qquad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix},$$

$$A = \begin{bmatrix} 0 & 0 \\ A & B \end{bmatrix}, \qquad U = \begin{bmatrix} I & 0 & 0 \\ 0 & \mu & e-\mu \end{bmatrix}, \qquad B = \begin{bmatrix} A & B \\ 0 & 0 \\ \nu^T & \omega^T \end{bmatrix}, \qquad V = \begin{bmatrix} I & \mu & e-\mu \\ 0 & 0 & I \\ 0 & 0 & I-\theta \end{bmatrix},$$

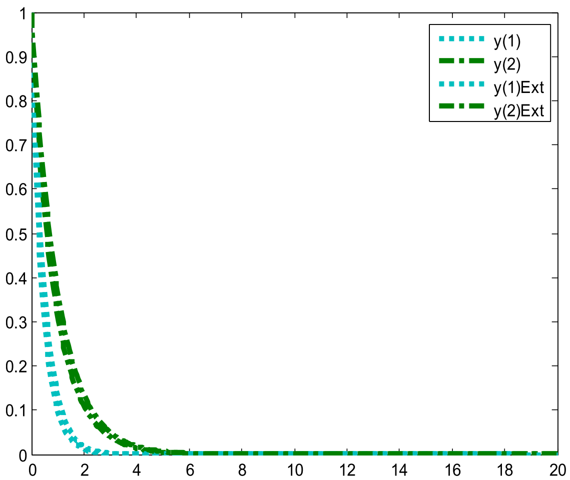
and $e = [1, \ldots, 1]^T \in R^m$.

Table 2
Absolute errors in the numerical integration of Example 1.

x	y_i	Method (3.2)	Method (3.4)
5	y_1	$4.68896460200918 \times 10^{-3}$	$5.82586126945793 \times 10^{-2}$
	y_2	$4.83268602450415 \times 10^{-3}$	$3.22595741549568 \times 10^{-2}$
50	y_1	$1.41564332474201 \times 10^{-2}$	$6.73587600368532 \times 10^{-3}$
	y_2	$1.94190326066295 \times 10^{-2}$	$2.61818804334955 \times 10^{-2}$
150	y_1	$6.38839815020812 \times 10^{-4}$	$2.46861111282455 \times 10^{-6}$
	y_2	$6.11344493813702 \times 10^{-3}$	$5.36087903326521 \times 10^{-4}$
250	y_1	$1.78956600076024 \times 10^{-5}$	$8.16360724925787 \times 10^{-10}$
	y_2	$1.22752851022732 \times 10^{-3}$	$9.75974730914864 \times 10^{-6}$
500	y_1	$1.60118070276548 \times 10^{-9}$	$1.61658927943642 \times 10^{-18}$
	y_2	$1.52678009269297 \times 10^{-5}$	$4.34316552414621 \times 10^{-10}$



Solution of example 1 using method (3.2), with nfe =500



Solution of example 1 using method (3.4), with nfe =500

Fig. 2. Graphical plots of Example 1 using the SDM methods.

Table 3
Absolute errors in the numerical integration of Example 2.

x	y_i	Method (3.2)	Method (3.4)
5	y_1	$4.40971863813200 \times 10^{-5}$	$6.66133814775094 \times 10^{-16}$
	y_2	$5.26519205076292 \times 10^{-5}$	$2.88657986402541 \times 10^{-15}$
	y_3	$3.85934636426555 \times 10^{-6}$	$8.88178419700125 \times 10^{-16}$
50	y_1	$1.78566343157632 \times 10^{-4}$	$7.35522753814166 \times 10^{-15}$
	y_2	$2.90906708941163 \times 10^{-4}$	$2.22044604925031 \times 10^{-15}$
	y_3	$1.91872056396480 \times 10^{-5}$	$9.99200722162641 \times 10^{-16}$
150	y_1	$6.90448713964037 \times 10^{-5}$	$1.74166236988071 \times 10^{-15}$
	y_2	$1.21583631077324 \times 10^{-4}$	$1.78329573330416 \times 10^{-15}$
	y_3	$7.86493242575792 \times 10^{-6}$	$1.08940634291343 \times 10^{-15}$
250	y_1	$3.14733754003677 \times 10^{-5}$	$1.49186218934005 \times 10^{-16}$
	y_2	$3.98514836908760 \times 10^{-7}$	$5.73759789679329 \times 10^{-16}$
	y_3	$1.77174473847859 \times 10^{-6}$	$2.26381413614973 \times 10^{-16}$
500	y_1	$1.87055194081974 \times 10^{-7}$	$7.63854311833928 \times 10^{-18}$
	y_2	$3.76170719057541 \times 10^{-7}$	$1.32814766129474 \times 10^{-18}$
	y_3	$2.36883627840876 \times 10^{-8}$	$3.59819595993627 \times 10^{-18}$

Hence (4.4a) takes the form

$$\begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \\ - \\ y_1^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} = \left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \begin{bmatrix} hf(Y_1^{[n]}) \\ hf(Y_2^{[n]}) \\ \vdots \\ hf(Y_s^{[n]}) \\ - \\ y_1^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \tag{4.4b}$$

where r denotes quantities as output from each step and input to the next step and s denotes stage values used in the computation of the step $y_1, y_2, \ldots, y_s$. The coefficients of these matrices indicate the relationship between the various numerical quantities that arise in the computation of stability regions. The elements of the matrices A, U, B and V are substituted into the stability matrix. In the sense of [26] we apply (4.4) to the linear test equation $y' = \lambda y, x \geq 0$ and $\lambda \in C$ but for the second-derivative high-order method we use $y'' = \lambda^2 y$, which leads to the recurrence relation $y^{[n+1]} = M(z)y^{[n]}, n = 1, 2, \ldots, N-1, z = \lambda h$, where the stability matrix $M(z)$ is defined by

$$M(z) = V + zB(1 - zA)^{-1}U. \tag{4.5}$$

We also define the stability polynomial $p(\eta, z)$ by the relation

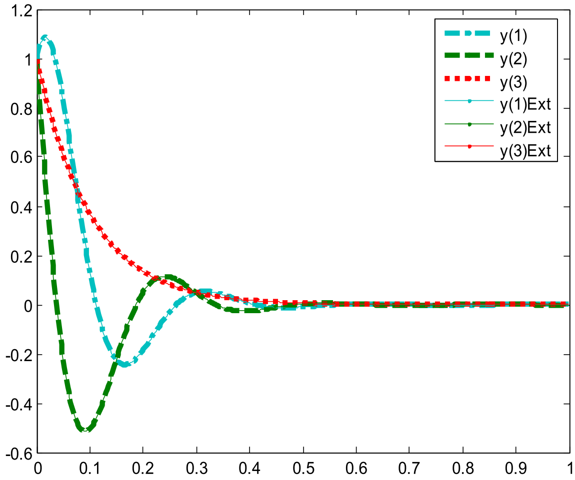
$$\rho(\eta,\ z) = \det(\eta I - M(z)) \tag{4.6}$$

and the absolute stability region $\Re$ of the method is given by

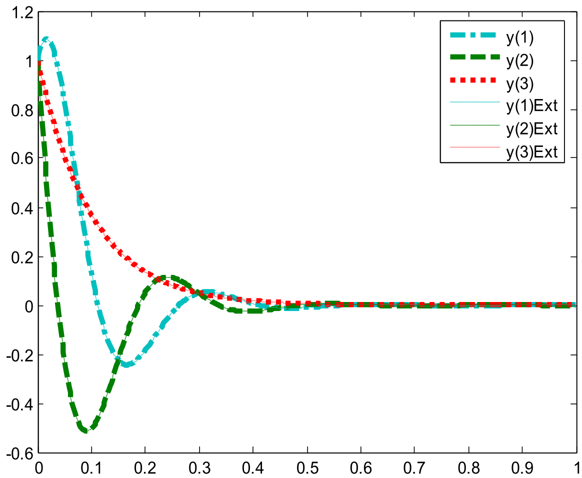
$$\Re = x \in C : \rho(\eta, z) = 1 \Rightarrow |\eta| \leq 1.$$

To compute the region of absolute stability we substitute the elements of the matrices A, U, B and V into the stability function (4.5) and finally into the stability polynomial (4.6) of the methods, which is plotted to produce the required graphs of the absolute stability regions of the methods as shown in Fig. 1.

The region of absolute stability of method (3.4) is A-stable, since the region consists of the complex plane outside the enclosed figure, but for method (3.2) it is $A(\alpha)$-stable.



Solution of example 2 using method (3.2), with nfe =500



Solution of example 2 using method (3.4), with nfe =500

Fig. 3. Graphical plots of Example 2 using the SDM methods.

5. Numerical examples

In this section, we present some numerical experiments on well-known stiff problems, intended to get insight about the performance of the second-derivative multistep methods. We have considered seven problems where the problems can be well integrated by using constant step-sizes. We present the computed results side by side in Tables in the formalism of Butcher and Hojjati [27]. We also show the efficiency curves for the problems considered. In the computation we use *nfe* to denote the number of function evaluations per step and *Ext* to indicate the exact solution.

Example 1 (*Stiff Nonlinear Problem (The Kaps Problem)*)**.** In the first example we consider stiff nonlinear system of two dimensional **Kaps** problem with corresponding initial conditions,

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \end{bmatrix} = \begin{bmatrix} -1002y_1(x) + 1000y_2(x)^2 \\ y_1(x) - y_2(x)(1 + y_2(x)) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

The exact solution is

$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} \exp(-2x) \\ \exp(-x) \end{bmatrix}.$$

Table 4
Absolute errors in the numerical integration of Example 3.

x	y_i	Method (3.2)	Method (3.4)
5	y_1	$4.14367031659202 \times 10^{-9}$	$5.03069808033274 \times 10^{-17}$
	y_2	$2.94649860066443 \times 10^{-11}$	$5.55111512312578 \times 10^{-16}$
	y_3	$1.08407556592693 \times 10^{-4}$	$5.88418203051333 \times 10^{-14}$
50	y_1	$5.05211923962356 \times 10^{-8}$	$3.60822483003176 \times 10^{-16}$
	y_2	$4.93082952246482 \times 10^{-9}$	$1.77635683940025 \times 10^{-15}$
	y_3	$1.39436797204684 \times 10^{-4}$	$3.06255021342849 \times 10^{-13}$
150	y_1	$1.47566447228353 \times 10^{-7}$	$2.22044604925031 \times 10^{-15}$
	y_2	$4.52747341839199 \times 10^{-8}$	$2.55351295663786 \times 10^{-15}$
	y_3	$2.97730144732666 \times 10^{-6}$	$3.32123217816616 \times 10^{-13}$
250	y_1	$2.26607868469841 \times 10^{-7}$	$1.44328993201270 \times 10^{-15}$
	y_2	$1.23235853521919 \times 10^{-7}$	0
	y_3	$2.58179316980911 \times 10^{-7}$	$3.06976666308856 \times 10^{-13}$
500	y_1	$2.79695260063662 \times 10^{-7}$	$3.77475828372553 \times 10^{-15}$
	y_2	$4.34733628873474 \times 10^{-7}$	$3.88578058618805 \times 10^{-15}$
	y_3	$2.79695490545961 \times 10^{-7}$	$1.98396854500515 \times 10^{-13}$

Table 5
Absolute errors in the numerical integration of Example 4.

x	y_i	Method (3.2)	Method (3.4)
5	y_1	$5.42017069791179 \times 10^{-5}$	$4.44089209850063 \times 10^{-16}$
	y_2	$5.42017064611988 \times 10^{-5}$	$5.55111512312578 \times 10^{-16}$
	y_3	$6.38528028060970 \times 10^{-4}$	$2.22044604925031 \times 10^{-16}$
50	y_1	$6.96931443209259 \times 10^{-5}$	$4.44089209850063 \times 10^{-15}$
	y_2	$6.96931380061161 \times 10^{-5}$	$9.29811783123569 \times 10^{-16}$
	y_3	$1.01845432154635 \times 10^{-4}$	$3.60822483003176 \times 10^{-16}$
150	y_1	$1.41488651017596 \times 10^{-6}$	$2.99760216648792 \times 10^{-15}$
	y_2	$1.41486750003593 \times 10^{-6}$	$2.25514051876985 \times 10^{-17}$
	y_3	$1.41546093522960 \times 10^{-6}$	$1.83230167150050 \times 10^{-17}$
250	y_1	$1.58171764574888 \times 10^{-8}$	$8.54871728961371 \times 10^{-15}$
	y_2	$1.57857242309277 \times 10^{-8}$	$2.58345048912562 \times 10^{-19}$
	y_3	$1.57857302506672 \times 10^{-8}$	$2.21922632180627 \times 10^{-19}$
500	y_1	$6.15847373097722 \times 10^{-11}$	$1.68753899743024 \times 10^{-14}$
	y_2	$1.15214011872475 \times 10^{-13}$	$1.96940071621512 \times 10^{-24}$
	y_3	$1.15214011872470 \times 10^{-13}$	$1.84338491977149 \times 10^{-24}$

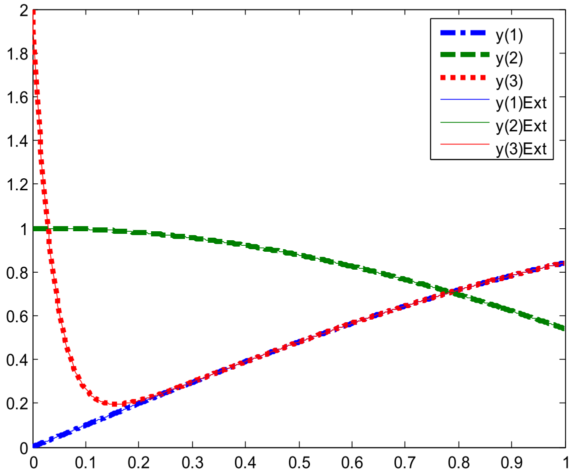
The computed solutions of this problem using the newly derived methods on the interval [0, 20] are shown in Table 2, while graphical plots are displayed in Fig. 2.

Example 2. The second test problem is a well-known classical system. It is a stiff linear problem composed of first order equations, with the initial conditions as follows

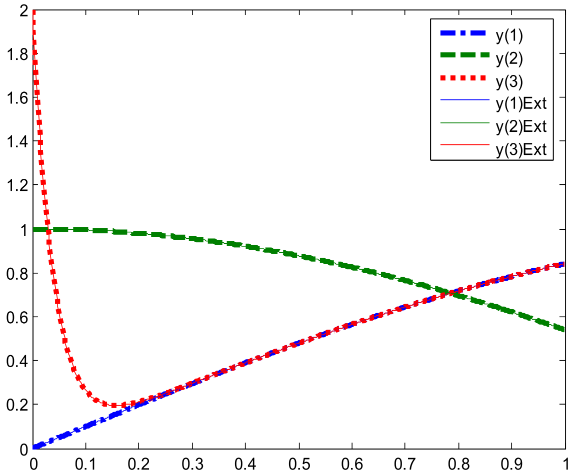
$$\begin{aligned} y_1'(x) &= -10y_1 + \beta y_2, & y_1(0) &= 1,\\ y_2'(x) &= -\beta y_1 - 10y_2, & y_2(0) &= 1,\\ y_3'(x) &= -\gamma y_3, & y_3(0) &= 1. \end{aligned}$$

The exact solution is given by

$$\begin{cases} y_1(x) = e^{-\gamma x}(\cos(\beta x) + \sin(\beta x)),\\ y_2(x) = e^{-\gamma x}(\cos(\beta x) - \sin(\beta x)),\\ y_3(x) = e^{-\gamma x}. \end{cases}$$



Solution of example 3 using Method (3.2), with nfe = 500



Solution of example 3 using method (3.4), with nfe = 500

Fig. 4. Graphical plots of Example 3 using SDM methods.

Table 6
Absolute errors in the numerical integration of Example 5.

x	y_i	Method (3.2)	Method (3.4)
	y_1	$5.66046680552379 \times 10^{-5}$	$5.02264896340421 \times 10^{-13}$
5	y_2	$5.66087578904514 \times 10^{-5}$	$5.12756503923129 \times 10^{-13}$
	y_3	$1.61778352103514 \times 10^{-5}$	$7.99749155788732 \times 10^{-13}$
	y_1	$4.19604912917926 \times 10^{-5}$	$5.35682609381638 \times 10^{-15}$
50	y_2	$4.19147028993261 \times 10^{-5}$	$9.99200722162641 \times 10^{-16}$
	y_3	$2.15757151141333 \times 10^{-4}$	$6.45874682732416 \times 10^{-15}$
	y_1	$2.49393655449293 \times 10^{-7}$	$1.56992474575901 \times 10^{-16}$
250	y_2	$9.34237112670822 \times 10^{-8}$	$4.25007251614318 \times 10^{-17}$
	y_3	$1.94078737508479 \times 10^{-7}$	$1.20548644599462 \times 10^{-16}$
	y_1	$9.47822290653377 \times 10^{-8}$	$1.53482370042479 \times 10^{-18}$
500	y_2	$9.47988235966424 \times 10^{-8}$	$7.58941520739853 \times 10^{-19}$
	y_3	$3.16824322296340 \times 10^{-11}$	$7.99539591804583 \times 10^{-19}$

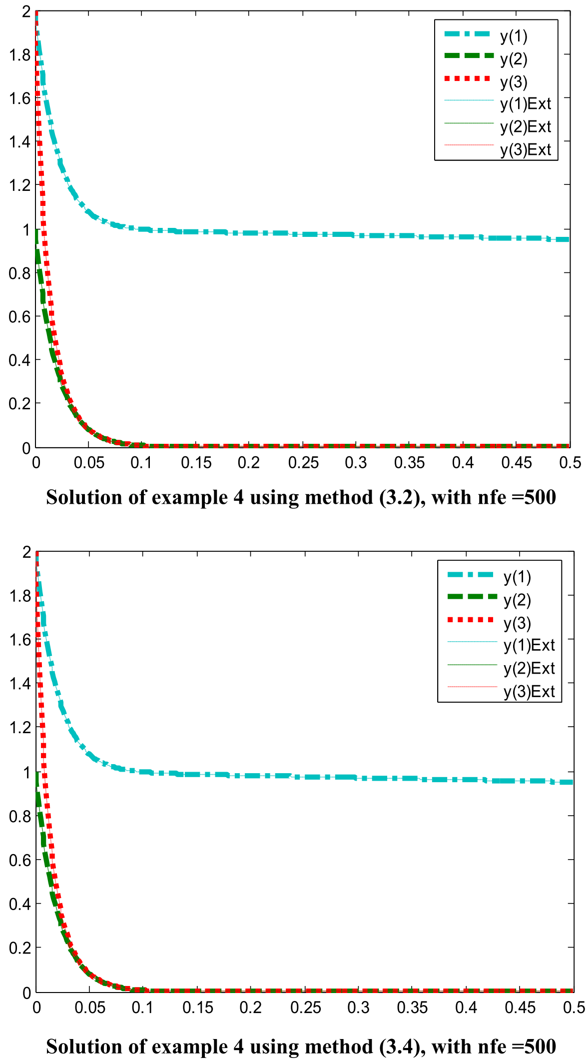


Fig. 5. Graphical plots of Example 4 using SDM methods.

The problem is integrated in the range [0, 1] and the results obtained are shown in Table 3, while the efficiency curves are displayed in Fig. 3.

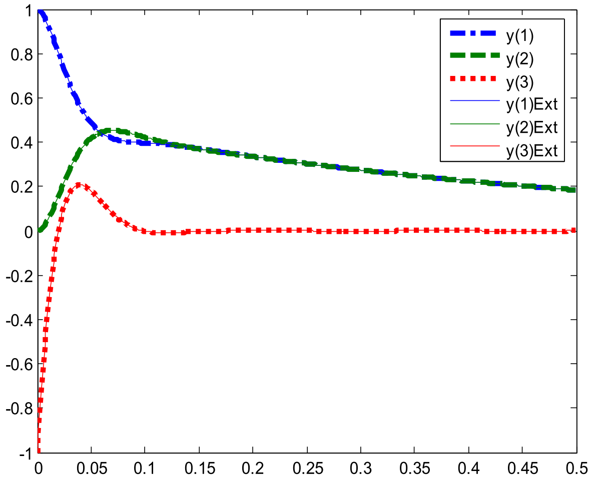
Example 3 (*Stiff Linear Problem*)**.** The third example is a linear stiff system of ordinary differential equations.

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \\ y_3'(x) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ -L & 1 & L \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ \ni \end{bmatrix}$$

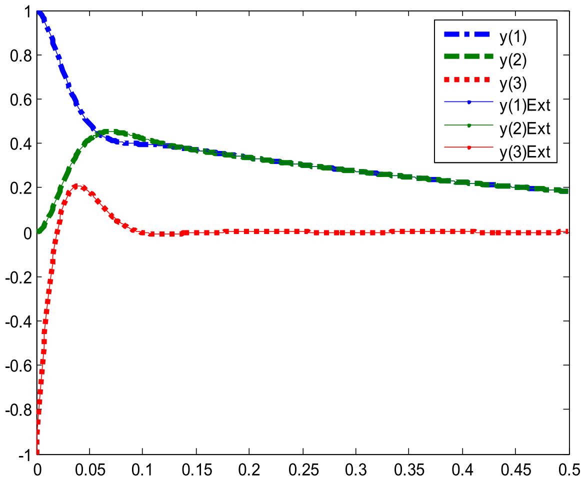
where $L = -25$ and $\ni= 2$. The exact solution is

$$\begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix} = \begin{bmatrix} \sin(x) \\ \cos(x) \\ \sin(x)+ \ni \exp(Lx) \end{bmatrix}.$$

This example is solved in the range of [0, 1] and the results obtained are presented in Table 4, while the efficiency curves are displayed in Fig. 4.



Solution of example 5 using method (3.2), with nfe =500



Solution of example 5 using method (3.4), with nfe =500

Fig. 6. Graphical plots of Example 5 using SDM methods.

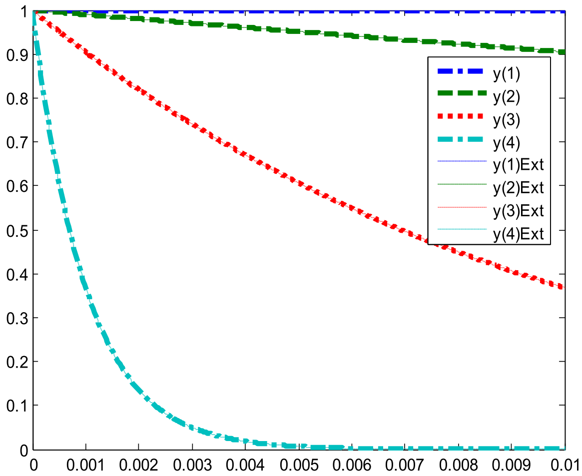
Example 4. In this example, we consider the stiff system with corresponding initial conditions:

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \\ y_3'(x) \end{bmatrix} = \begin{bmatrix} -0.1 & 49.9 & 0 \\ 0 & -50 & 0 \\ 0 & 70 & -120 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}.$$

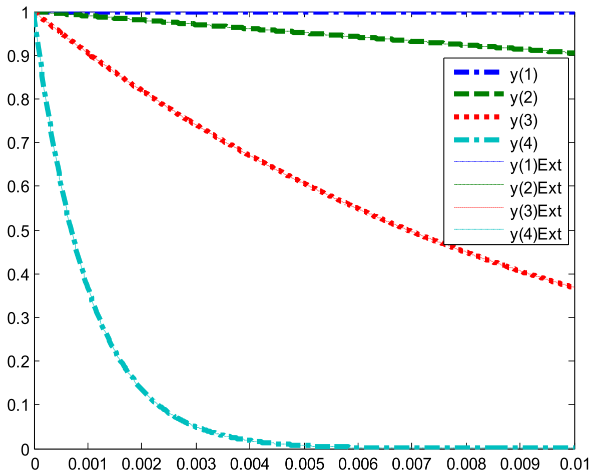
The exact solution is

$$\begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix} = \begin{bmatrix} \exp(-0.1x) + \exp(-50x) \\ \exp(-50x) \\ \exp(-50x) + \exp(-120x) \end{bmatrix}.$$

In Table 5, the computed solutions of the problem using the new methods on the interval of [0, 0.5] are shown side by side. From this example, it is clearly confirmed that the second-derivative high-order accuracy methods are appropriate for stiff problems (see Figs. 2–8).



Solution of example 6 using method (3.2), with nfe =500



Solution of example 6 using method (3.4), with nfe =500

Fig. 7. Graphical plots of Example 6 using SDM methods.

Example 5. The fifth example is a highly stiff system (see Lambert [28])

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \\ y_3'(x) \end{bmatrix} = \begin{bmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}.$$

The exact solution is

$$\begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix} = \begin{bmatrix} 0.5\exp(-2x) + 0.5\exp(-40x)(\cos 40x + \sin 40x) \\ 0.5\exp(-2x) - 0.5\exp(-40x)(\cos 40x + \sin 40x) \\ -\exp(-40x)(\cos 40x + \sin 40x) \end{bmatrix}.$$

We solve the problem in the range [0, 0.5] and the computed results are shown in Table 6.

Example 6. The linear problem by Enright [8] is solved:

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \\ y_3'(x) \\ y_4'(x) \end{bmatrix} = \begin{bmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \\ y_4(x) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \\ y_4(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

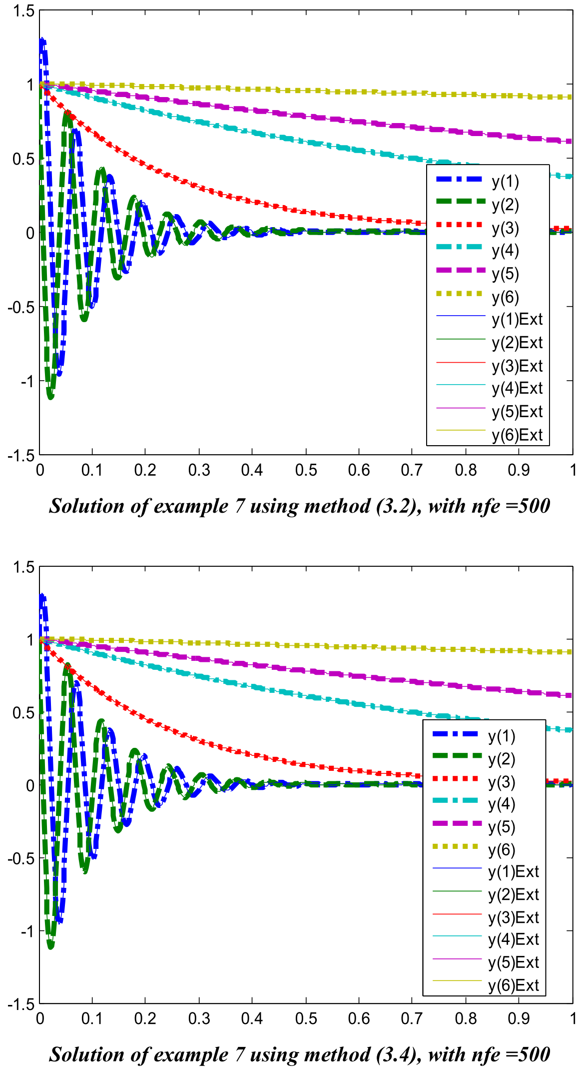


Fig. 8. Graphical plots of Example 7 using SDM methods.

This problem was integrated using the newly constructed methods. In Table 7 we list the results obtained at the end point of the range of integration [0, 0.1].

Example 7. Finally, we consider another linear problem which is particularly referred to by Fatunla [29] as a troublesome problem. This is because some of the eigenvalues lying close to the imaginary axis, a case where some stiff integrators were known to be inefficient. These eigenvalues of the Jacobian are $\lambda_{1,2} = -10 \pm 100i$, $\lambda_3 = -4$, $\lambda_4 = -1$, $\lambda_5 = -0.5$ and $\lambda_6 = -0.1$.

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \\ y_3'(x) \\ y_4'(x) \\ y_5'(x) \\ y_6'(x) \end{bmatrix} = \begin{bmatrix} -10 & 100 & 0 & 0 & 0 & 0 \\ -100 & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.1 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \\ y_4(x) \\ y_5(x) \\ y_6(x) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \\ y_4(0) \\ y_5(0) \\ y_6(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

This problem is solved within the interval of [0, 1], thus, only the first four components of the solutions are shown in the Table 8 $\{y_1, y_2, y_3, y_4\}$.

Table 7
Absolute errors in the numerical integration of Example 6.

x	y_i	Method (3.2)	Method (3.4)
5	y_1	0	0
	y_2	$4.14090983724691 \times 10^{-12}$	$6.66133814775094 \times 10^{-16}$
	y_3	$4.11441414271962 \times 10^{-9}$	$4.44089209850063 \times 10^{-16}$
	y_4	$3.85934636437657 \times 10^{-6}$	$9.99200722162641 \times 10^{-16}$
50	y_1	$4.44089209850063 \times 10^{-16}$	$3.66373598126302 \times 10^{-15}$
	y_2	$5.02700103766074 \times 10^{-11}$	$8.88178419700125 \times 10^{-16}$
	y_3	$4.60552629366617 \times 10^{-8}$	0
	y_4	$1.91872056397036 \times 10^{-5}$	$2.22044604925031 \times 10^{-16}$
250	y_1	$5.55111512312578 \times 10^{-16}$	$1.06581410364015 \times 10^{-14}$
	y_2	$2.45416020838718 \times 10^{-10}$	$5.55111512312578 \times 10^{-16}$
	y_3	$1.56753285796007 \times 10^{-7}$	$6.77236045021345 \times 10^{-15}$
	y_4	$1.77174473848119 \times 10^{-6}$	$2.77555756156289 \times 10^{-17}$
500	y_1	$5.55111512312578 \times 10^{-16}$	$6.32827124036339 \times 10^{-15}$
	y_2	$4.67785365998452 \times 10^{-10}$	$4.44089209850063 \times 10^{-15}$
	y_3	$1.90342383799003 \times 10^{-7}$	$8.77076189453874 \times 10^{-15}$
	y_4	$2.36883627840470 \times 10^{-8}$	$1.35525271560688 \times 10^{-19}$

Table 8
Absolute errors in the numerical integration of Example 7.

x	y_i	Method (3.2)	Method (3.4)
5	y_1	$1.24324315198199 \times 10^{-3}$	$2.22044604925031 \times 10^{-16}$
	y_2	$5.39904813468630 \times 10^{-3}$	$1.74166236988071 \times 10^{-15}$
	y_3	$2.57764644295833 \times 10^{-7}$	$3.33066907387547 \times 10^{-16}$
	y_4	$4.11441414271962 \times 10^{-9}$	$2.22044604925031 \times 10^{-16}$
50	y_1	$4.28744995223446 \times 10^{-3}$	$1.66533453693773 \times 10^{-15}$
	y_2	$2.70680071784902 \times 10^{-2}$	$8.24340595784179 \times 10^{-15}$
	y_3	$2.20140908635535 \times 10^{-6}$	$2.55351295663786 \times 10^{-15}$
	y_4	$4.60552630476840 \times 10^{-8}$	$3.77475828372553 \times 10^{-15}$
250	y_1	$1.79667994879615 \times 10^{-3}$	$5.86336534880161 \times 10^{-16}$
	y_2	$1.69369470423685 \times 10^{-3}$	$4.18068357710411 \times 10^{-16}$
	y_3	$2.25135101852847 \times 10^{-6}$	$3.63598040564739 \times 10^{-15}$
	y_4	$1.56753285907030 \times 10^{-7}$	$5.10702591327572 \times 10^{-15}$
500	y_1	$2.40165186584563 \times 10^{-5}$	$8.73121562029733 \times 10^{-18}$
	y_2	$2.09323599425030 \times 10^{-5}$	$4.43167638003450 \times 10^{-18}$
	y_3	$6.08160768331839 \times 10^{-7}$	$8.15320033709099 \times 10^{-16}$
	y_4	$1.90342383910025 \times 10^{-7}$	$1.66533453693773 \times 10^{-16}$

Concluding remarks

We subjected the newly derived methods to detailed implementations using stiff systems of ordinary different equations. The methods so constructed in this paper perform well on stiff systems found in the literature. The results from the new high-order methods are very promising therefore encouraging further investigation of the second-derivative type of methods is necessary, particularly the upgraded method which outperformed the non-upgraded method in all the examples considered in the paper.

Acknowledgments

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